

# ATOMISTICALLY-INFORMED COHESIVE ZONE LAWS: A METHODOLOGY FOR LINKING CHEMICAL BONDING WITH PLASTICITY

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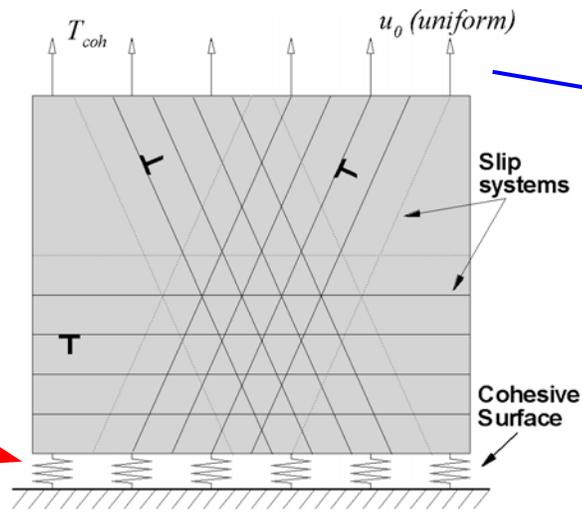
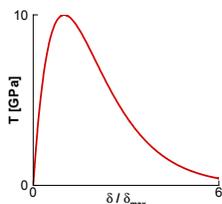
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The maximum stress predicted from an atomic-scale calculation of tensile debonding at a material interface is generally several orders-of-magnitude larger than what is observed in practice. One possible explanation for this pertains to the absence of mechanical defects, such as dislocations, in the atomistic calculations. To explore this issue, we present a methodology with which cohesive zone laws used in continuum models of plasticity and fracture can be informed with chemical bonding information from atomistic-scale calculations and mesoscale information on the effect of mechanical defects. Two cohesive zone laws generated from atomistic tensile debonding calculations of the Al(111)/diamond(111)1x1 and Al(111)/diamond(111)2x1 interfaces are used as interfacial constitutive laws in a discrete dislocation analysis of an fcc material (i.e. Aluminum) bound to a rigid material (i.e. diamond). Cohesive laws are generated from the results of this analysis that include the effects of dislocation nucleation, motion, and interaction with obstacles on the apparent cohesive strength and cohesive energy.

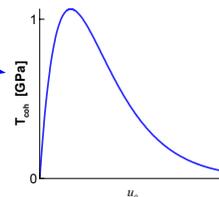
## Input:

From atomistic simulations



## Output:

To continuum scale



**Figure:** Bridging between atomic surface properties and continuum cohesive properties.